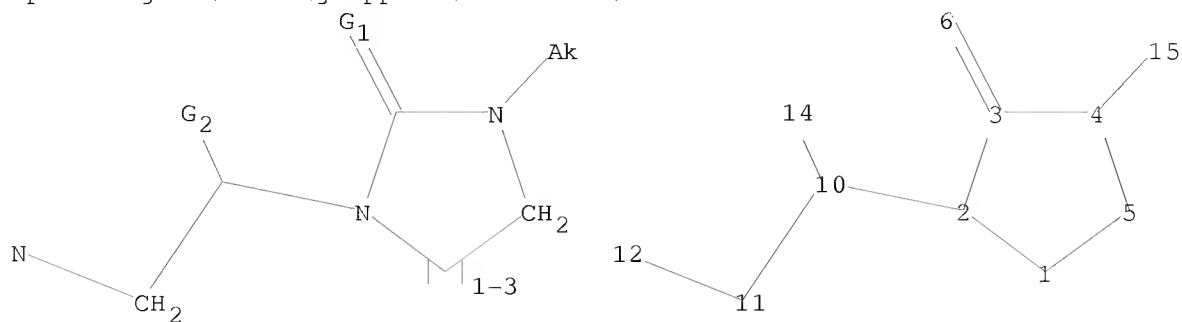


Uploading C:\Users\jcoppins\Documents\10593941.str



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chain nodes :
6 10 11 12 14 15
ring nodes :
1 2 3 4 5
chain bonds :
2-10 3-6 4-15 10-11 10-14 11-12
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-15 10-14
exact bonds :
10-11 11-12

```

G1:O,S,N

G2:H,Ak

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 10:CLASS 11:CLASS 12:CLASS
14:CLASS
15:CLASS

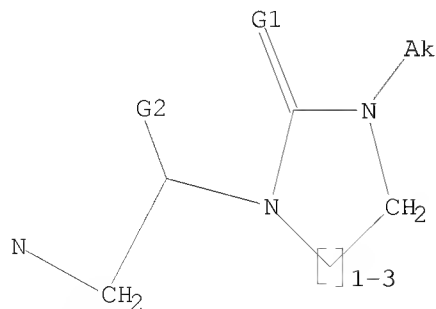
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L1 STRUCTURE UPLOADED

=> d

L1 HAS NO ANSWERS

L1 STR



G1:O,S,N

G2:H,Ak

Structure attributes must be viewed using STN Express query preparation.

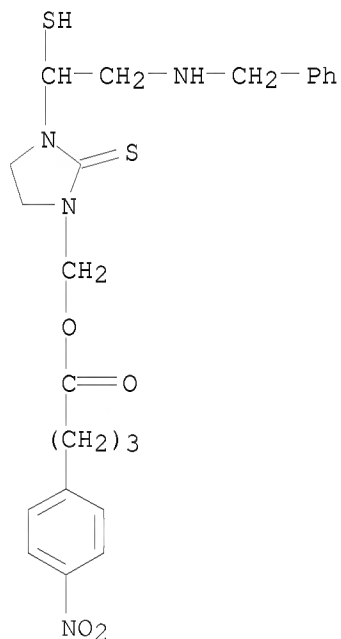
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FULL SCREEN SEARCH COMPLETED - 240363 TO ITERATE

100.0% PROCESSED 240363 ITERATIONS 215 ANSWERS  
SEARCH TIME: 00.00.03

L2 215 SEA SSS FUL L1

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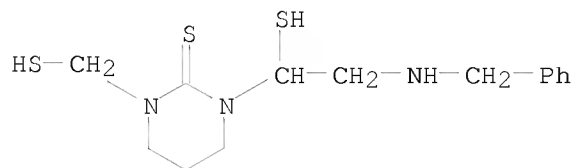
L2 ANSWER 1 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1349551-98-9 REGISTRY  
ED Entered STN: 06 Dec 2011  
CN Benzenebutanoic acid, 4-nitro-, [3-[1-mercapto-2-  
[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA  
INDEX NAME)  
MF C23 H28 N4 O4 S2  
SR Other Sources  
Database: GVK BIO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

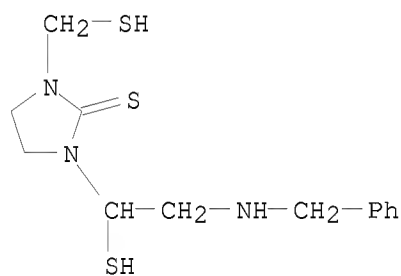
L2 ANSWER 2 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1348962-28-6 REGISTRY  
ED Entered STN: 05 Dec 2011

CN 2(1H)-Pyrimidinethione, tetrahydro-1-(mercaptomethyl)-3-[1-mercapto-2-  
 [(phenylmethyl)amino]ethyl]- (CA INDEX NAME)  
 MF C14 H21 N3 S3  
 SR Other Sources  
 Database: GVK BIO



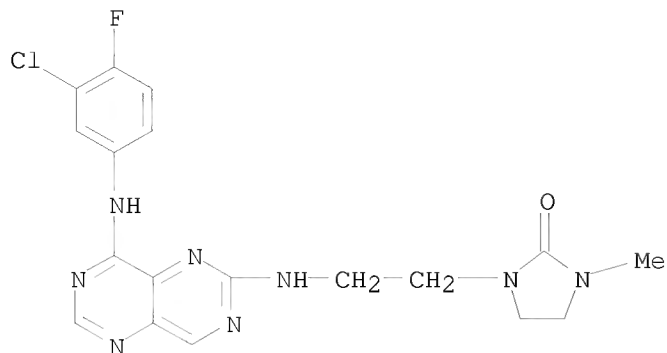
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 3 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348828-94-3 REGISTRY  
 ED Entered STN: 05 Dec 2011  
 CN 2-Imidazolidinethione, 1-(mercaptomethyl)-3-[1-mercapto-2-  
 [(phenylmethyl)amino]ethyl]- (CA INDEX NAME)  
 MF C13 H19 N3 S3  
 SR Other Sources  
 Database: GVK BIO



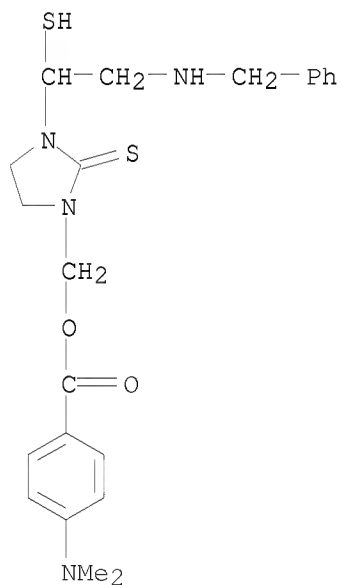
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 4 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348799-25-6 REGISTRY  
 ED Entered STN: 05 Dec 2011  
 CN 2-Imidazolidinone, 1-[2-[[8-[(3-chloro-4-fluorophenyl)amino]pyrimido[5,4-  
 d]pyrimidin-2-yl]amino]ethyl]-3-methyl- (CA INDEX NAME)  
 MF C18 H18 Cl F N8 O  
 SR Other Sources  
 Database: GVK BIO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

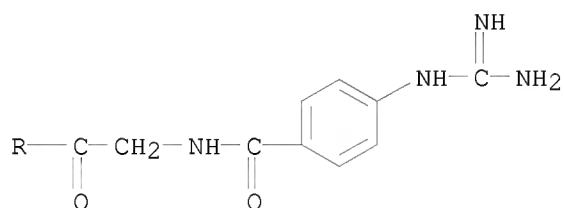
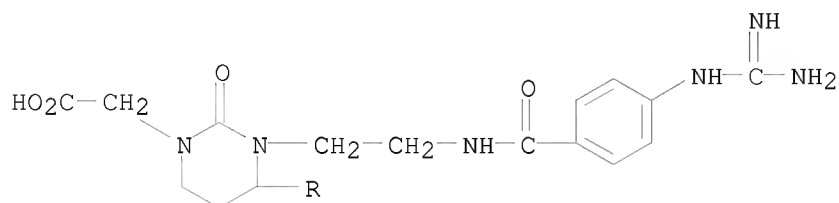
L2 ANSWER 5 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348516-48-2 REGISTRY  
 ED Entered STN: 04 Dec 2011  
 CN Benzoic acid, 4-(dimethylamino)-, [3-[1-mercapto-2-  
 [(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA  
 INDEX NAME)  
 MF C22 H28 N4 O2 S2  
 SR Other Sources  
 Database: GVK BIO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 ANSWER 6 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN

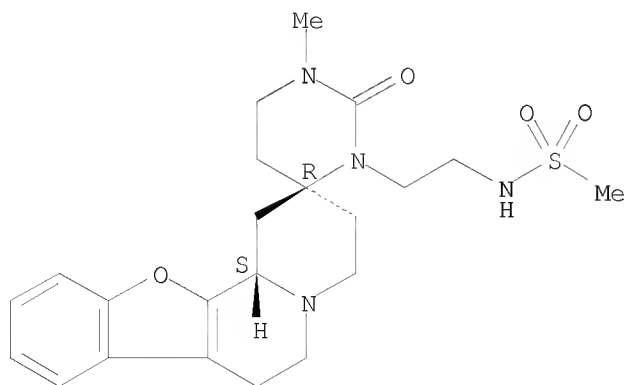
RN 1348070-78-9 REGISTRY  
 ED Entered STN: 04 Dec 2011  
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 [(aminoiminomethyl)amino]benzoyl]amino]acetyl]-3-[2-[[4-  
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 NAME)  
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 SR Other Sources  
 Database: GVK BIO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

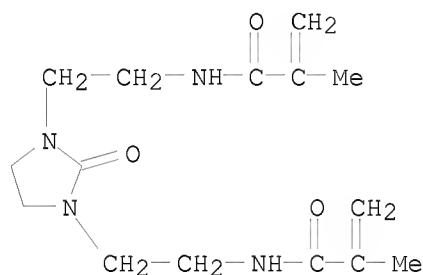
L2 ANSWER 7 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1347405-85-9 REGISTRY  
 ED Entered STN: 02 Dec 2011  
 CN INDEX NAME NOT YET ASSIGNED  
 FS STEREOSEARCH  
 MF C22 H30 N4 O4 S  
 SR Other Sources  
 Database: GVK BIO

Absolute stereochemistry.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

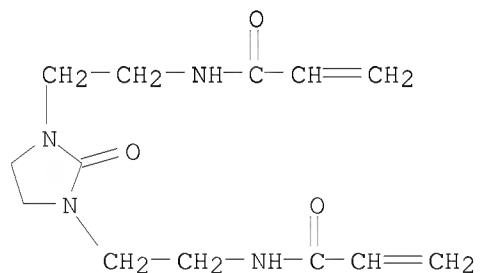
L2 ANSWER 8 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1346551-34-5 REGISTRY  
ED Entered STN: 29 Nov 2011  
CN INDEX NAME NOT YET ASSIGNED  
MF C15 H24 N4 O3  
SR CA  
LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 9 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1346551-32-3 REGISTRY  
ED Entered STN: 29 Nov 2011  
CN INDEX NAME NOT YET ASSIGNED  
MF C13 H20 N4 O3  
SR CA  
LC STN Files: CA, CAPLUS

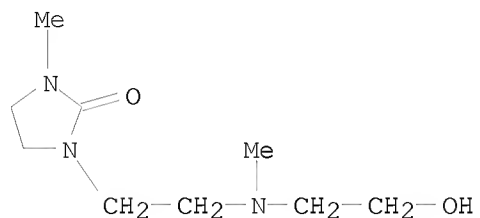


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L2 ANSWER 10 OF 215 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1315512-37-8 REGISTRY  
 ED Entered STN: 09 Aug 2011  
 CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA  
 INDEX NAME)  
 MF C9 H19 N3 O2  
 SR CA  
 LC STN Files: CA, CAPLUS, TOXCENTER

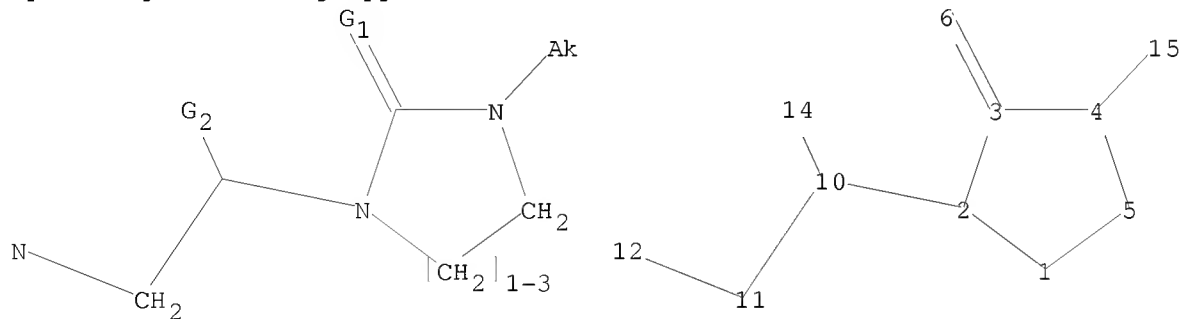


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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Uploading C:\Users\jcoppins\Documents\10593941a.str



chain nodes :  
 6 10 11 12 14 15  
 ring nodes :  
 1 2 3 4 5  
 chain bonds :  
 2-10 3-6 4-15 10-11 10-14 11-12  
 ring bonds :  
 1-2 1-5 2-3 3-4 4-5  
 exact/norm bonds :  
 1-2 1-5 2-3 2-10 3-4 3-6 4-5 4-15 10-14  
 exact bonds :  
 10-11 11-12

G1:O,S,N

G2:H,Ak

Match level :

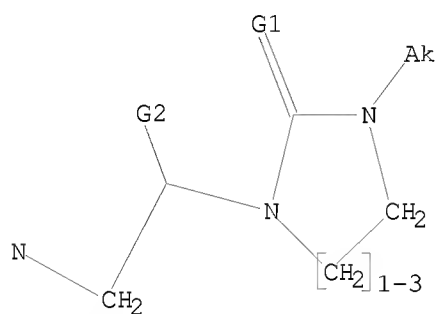
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 10:CLASS 11:CLASS 12:CLASS  
14:CLASS  
15:CLASS

L3 STRUCTURE UPLOADED

=> d

L3 HAS NO ANSWERS

L3 STR



G1:O, S, N

G2:H,Ak

Structure attributes must be viewed using STN Express query preparation.

=> s l3 ful

FULL SEARCH INITIATED 20:30:28 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 240363 TO ITERATE

100.0% PROCESSED 240363 ITERATIONS

175 ANSWERS

SEARCH TIME: 00.00.04

L4 175 SEA SSS FUL L3

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L4 ANSWER 1 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN

RN 1349551-98-9 REGISTRY

ED Entered STN: 06 Dec 2011

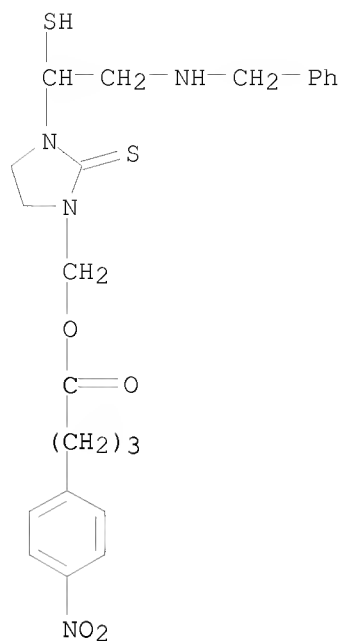
CN Benzenebutanoic acid, 4-nitro-, [3-[1-mercapto-2-  
[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA  
INDEX NAME)

MF C23 H28 N4 O4 S2

SR Other Sources

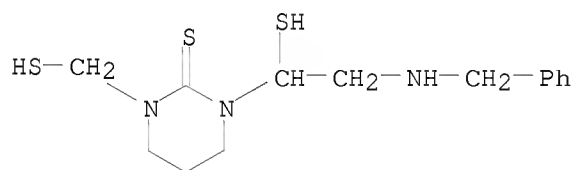
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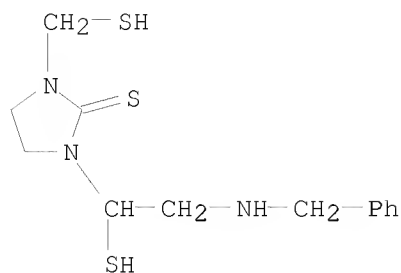
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 2 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348962-28-6 REGISTRY  
 ED Entered STN: 05 Dec 2011  
 CN 2(1H)-Pyrimidinethione, tetrahydro-1-(mercaptomethyl)-3-[1-mercapto-2-  
 [(phenylmethyl)amino]ethyl]- (CA INDEX NAME)  
 MF C14 H21 N3 S3  
 SR Other Sources  
 Database: GVK BIO



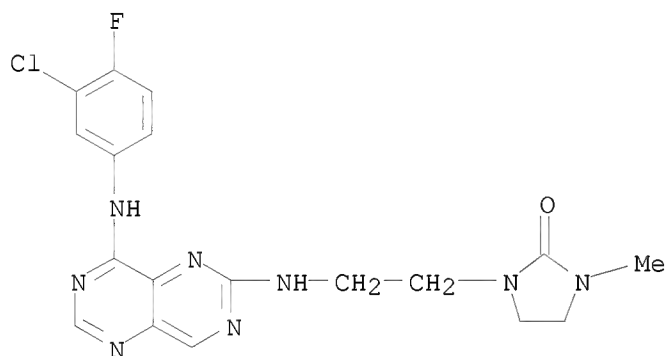
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 3 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348828-94-3 REGISTRY  
 ED Entered STN: 05 Dec 2011  
 CN 2-Imidazolidinethione, 1-(mercaptomethyl)-3-[1-mercapto-2-  
 [(phenylmethyl)amino]ethyl]- (CA INDEX NAME)  
 MF C13 H19 N3 S3  
 SR Other Sources  
 Database: GVK BIO



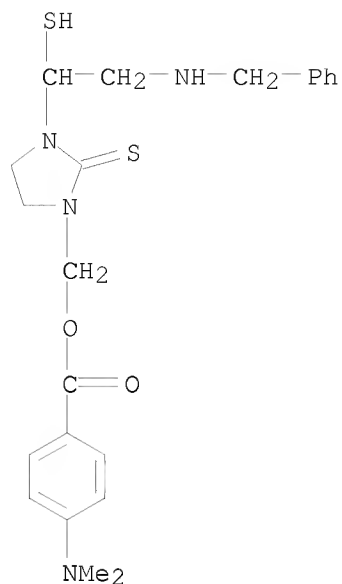
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 4 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348799-25-6 REGISTRY  
 ED Entered STN: 05 Dec 2011  
 CN 2-Imidazolidinone, 1-[2-[[8-[(3-chloro-4-fluorophenyl)amino]pyrimido[5,4-d]pyrimidin-2-yl]amino]ethyl]-3-methyl- (CA INDEX NAME)  
 MF C18 H18 Cl F N8 O  
 SR Other Sources  
 Database: GVK BIO



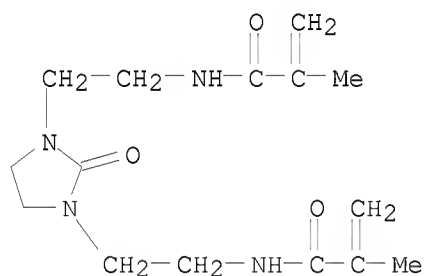
\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 5 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1348516-48-2 REGISTRY  
 ED Entered STN: 04 Dec 2011  
 CN Benzoic acid, 4-(dimethylamino)-, [3-[1-mercapto-2-[(phenylmethyl)amino]ethyl]-2-thioxo-1-imidazolidinyl]methyl ester (CA INDEX NAME)  
 MF C22 H28 N4 O2 S2  
 SR Other Sources  
 Database: GVK BIO



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L4 ANSWER 6 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1346551-34-5 REGISTRY  
 ED Entered STN: 29 Nov 2011  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C15 H24 N4 O3  
 SR CA  
 LC STN Files: CA, CAPLUS

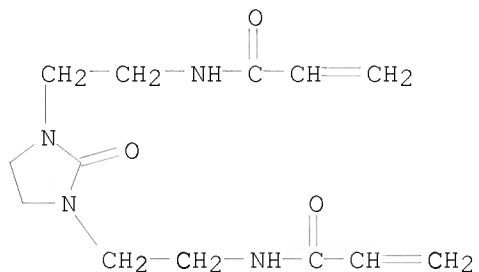


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 7 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
 RN 1346551-32-3 REGISTRY  
 ED Entered STN: 29 Nov 2011  
 CN INDEX NAME NOT YET ASSIGNED  
 MF C13 H20 N4 O3

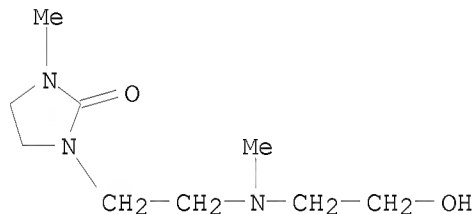
SR CA  
LC STN Files: CA, CAPLUS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 8 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1315512-37-8 REGISTRY  
ED Entered STN: 09 Aug 2011  
CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA INDEX NAME)  
MF C9 H19 N3 O2  
SR CA  
LC STN Files: CA, CAPLUS, TOXCENTER

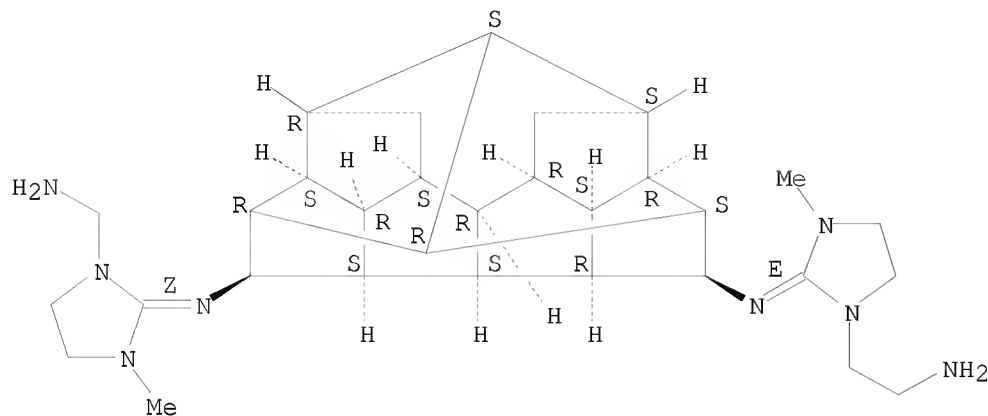


\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 9 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1261062-12-7 REGISTRY  
ED Entered STN: 28 Jan 2011  
CN 2,7,3,6-Ethanediylienedipentaleno[1,6-ab:1',6'-ef]pentalene-1,8-diamine, N1-[1-(2-aminoethyl)-3-methyl-2-imidazolinyliidene]-N8-[1-(aminomethyl)-3-methyl-2-imidazolinyliidene]octadecahydro-, stereoisomer (CA INDEX NAME)  
FS STEREOSEARCH  
MF C31 H46 N8  
SR CA  
LC STN Files: CA, CAPLUS

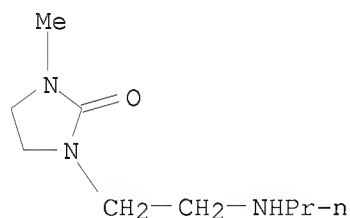
Relative stereochemistry.  
Double bond geometry as shown.



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)  
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L4 ANSWER 10 OF 175 REGISTRY COPYRIGHT 2011 ACS on STN  
RN 1250017-79-8 REGISTRY  
ED Entered STN: 01 Nov 2010  
CN 2-Imidazolidinone, 1-methyl-3-[2-(propylamino)ethyl]- (CA INDEX NAME)  
MF C9 H19 N3 O  
SR Chemical Catalog  
Supplier: Ukrorgsyntez Ltd.  
LC STN Files: CHEMCATS



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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COST IN U.S. DOLLARS  
FULL ESTIMATED COST

SINCE FILE	TOTAL
ENTRY	SESSION
440.80	441.03

FILE 'CAPLUS' ENTERED AT 20:31:42 ON 14 DEC 2011  
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
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FILE COVERS 1907 - 14 Dec 2011 VOL 155 ISS 25  
FILE LAST UPDATED: 13 Dec 2011 (20111213/ED)  
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2011  
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2011

CAPLUS now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2011.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 14

L5 61 L4

=> d 15 1-10 ibib abs hitstr

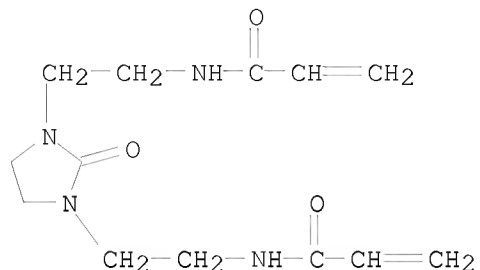
L5 ANSWER 1 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
ACCESSION NUMBER: 2011:1427380 CAPLUS <<LOGINID::20111214>>  
DOCUMENT NUMBER: 155:639066  
TITLE: Semi-acrylic polyurethane aqueous coating compositions with good adhesion and scratch and chemical resistance  
INVENTOR(S): Choi, Myeong Gi; Yang, Ji Won; Lim, Myeong Hyeok; Lee, Deok Hui  
PATENT ASSIGNEE(S): KCC Corp., S. Korea  
SOURCE: Repub. Korean Kongkae Taeho Kongbo, 7pp.  
CODEN: KRXXA7  
DOCUMENT TYPE: Patent  
LANGUAGE: Korean  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	KR 2011120610	A	20111104	KR 2010-40091	20100429
PRIORITY APPLN. INFO.:				KR 2010-40091	20100429
AB	Title compns. contain a chlorinated polyolefin, an acrylic polyolefin, a film-forming resin, a water-dispersible polyurethane, and a crosslinking agent.				
IT	1346551-32-3DP, polymers with polyolefin acrylate				
	RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)				
	(blend with chlorinated polyolefin and polyurethane; semi-acrylic				

polyurethane aqueous coating compns. with good adhesion and scratch and chemical resistance)

RN 1346551-32-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



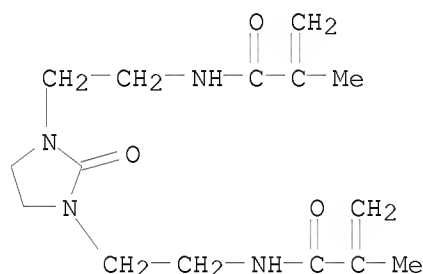
IT 1346551-34-5DP, polymers with polyolefin acrylate

RL: IMF (Industrial manufacture); POF (Polymer in formulation); PRP (Properties); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(semi-acrylic polyurethane aqueous coating compns. with good adhesion and scratch and chemical resistance)

RN 1346551-34-5 CAPLUS

CN INDEX NAME NOT YET ASSIGNED



L5 ANSWER 2 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2011:740834 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 155:250356

TITLE: Degradation of MMEA at absorber and stripper conditions

AUTHOR(S): Lepaumier, Helene; Grimstvedt, Andreas; Vernstad, Kai; Zahlse, Kolbjorn; Svendsen, Hallvard F.

CORPORATE SOURCE: Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Trondheim, N-7491, Norway

SOURCE: Chemical Engineering Science (2011), 66(15), 3491-3498  
CODEN: CESCAC; ISSN: 0009-2509

PUBLISHER: Elsevier Ltd.

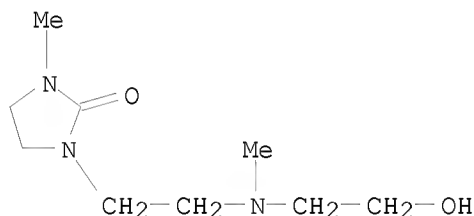
DOCUMENT TYPE: Journal; (online computer file)

LANGUAGE: English

AB This study examines the degradation of N-methylethanolamine (MMEA) under different exptl. conditions. Thermal degradation with and without CO<sub>2</sub>, and oxidative degradation are studied. Samples of the degraded solution were taken

at regular intervals and analyzed. The percentage of amine loss was determined by liquid chromatog.-mass spectrometry (LC-MS) while the degradation compds. were identified and quantified by gas chromatog.-mass spectrometry (GC-MS). MMEA degradation at absorber and stripper conditions is compared with previous work on 2-ethanolamine (MEA). Degradation mechanisms are proposed and discussed in order to understand the differences compared to MEA.

IT 1315512-37-8  
 RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)  
 (degradation of methylethanolamine at absorber and stripper conditions)  
 RN 1315512-37-8 CAPLUS  
 CN 2-Imidazolidinone, 1-[2-[(2-hydroxyethyl)methylamino]ethyl]-3-methyl- (CA INDEX NAME)



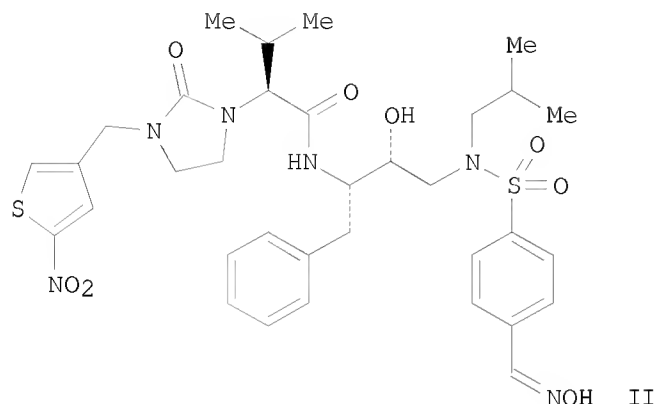
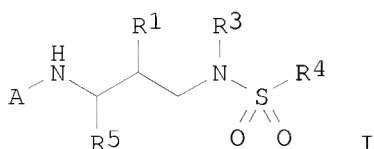
REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2011:20015 CAPLUS <<LOGINID::20111214>>  
 DOCUMENT NUMBER: 154:132821  
 TITLE: Preparation of sulfonylaminobutanamide derivatives for use as HIV protease inhibitors  
 INVENTOR(S): Flentge, Charles A.; Chen, Hui-Ju; Degoey, David A.; Flosi, William J.; Grampovnik, David J.; Huang, Peggy P.; Kempf, Dale J.; Klein, Larry L.; Krueger, Allan C.; Madigan, Darold L.; Randolph, John T.; Sun, Minghua; Yeung, Ming C.; Zhao, Chen  
 PATENT ASSIGNEE(S): Abbott Laboratories, USA  
 SOURCE: U.S. Pat. Appl. Publ., 230pp.  
 CODEN: USXXCO  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20110003827	A1	20110106	US 2004-9841	20041210
PRIORITY APPLN. INFO.:			US 2003-529121P	P 20031211
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT				
OTHER SOURCE(S):		MARPAT 154:132821		

GI





AB Title compds. I [A = C(O)alkyl, (un)substituted SO<sub>2</sub>-aryl, SO<sub>2</sub>-heteroaryl, etc.; R<sub>1</sub> = OH, OSO<sub>2</sub>H, OP(O)<sub>3</sub>H, etc.; R<sub>3</sub> = (un)substituted cycloalkyl, aryl, heteroaryl, etc.; R<sub>4</sub> = (un)substituted cycloalkyl, cycloalkenyl, heterocyclyl, aryl, or heteroaryl; R<sub>5</sub> = (un)substituted alkyl, alkenyl, cycloalkyl, arylalkyl, etc.], and their pharmaceutically acceptable salts, are prepared and disclosed as HIV protease inhibitors. Thus, e.g., II was prepared by a multistep procedure (preparation given). I were evaluated for activity against wild-type HIV or the passaged variants and demonstrated EC<sub>50</sub> values in the range of 1 nM to 100 nM.

IT 854742-89-5P 854742-90-8P

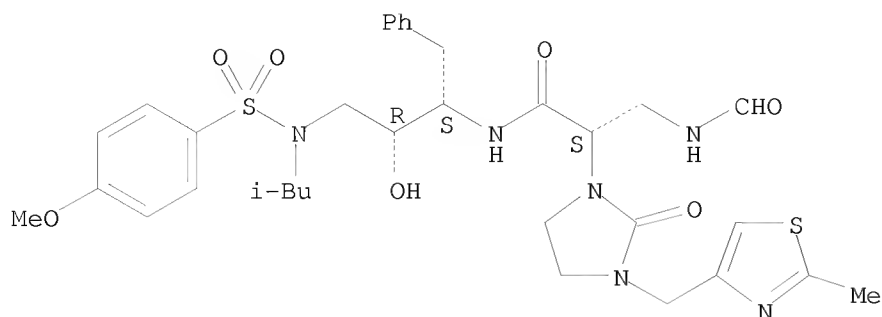
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of sulfonylaminobutanamide derivs. for use as HIV protease inhibitors)

RN 854742-89-5 CAPLUS

CN 1-Imidazolidineacetamide,  $\alpha$ -[(formylamino)methyl]-N-[(1S,2R)-2-hydroxy-3-[[4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-, ( $\alpha$ S)- (CA INDEX NAME)

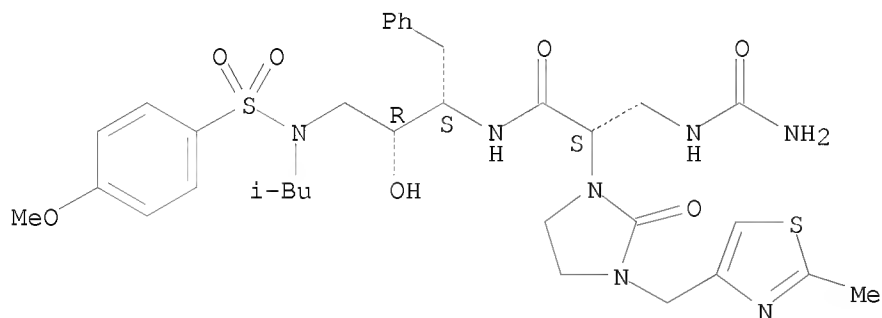
Absolute stereochemistry.



RN 854742-90-8 CAPLUS

CN 1-Imidazolidineacetamide,  $\alpha$ -[[[(aminocarbonyl)amino]methyl]-N-[(1S,2R)-2-hydroxy-3-[[[(4-methoxyphenyl)sulfonyl](2-methylpropyl)amino]-1-(phenylmethyl)propyl]-3-[(2-methyl-4-thiazolyl)methyl]-2-oxo-, ( $\alpha$ S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 1056133-73-3P 1056133-74-4P

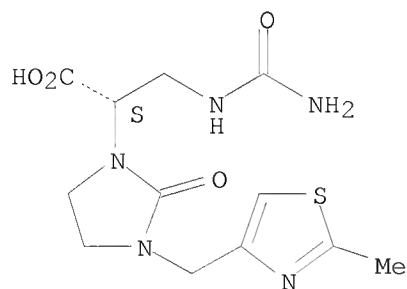
RL: PRPH (Prophetic); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of sulfonylaminobutanamide derivs. for use as HIV protease inhibitors)

RN 1056133-73-3 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Absolute stereochemistry.

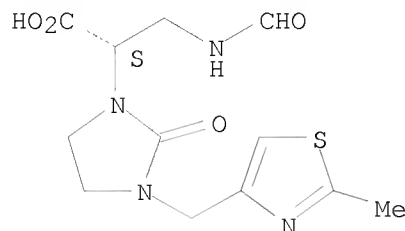


RN 1056133-74-4 CAPLUS

CN 1-Imidazolidineacetic acid,  $\alpha$ -[(formylamino)methyl]-3-[(2-methyl-4-

thiazolyl)methyl]-2-oxo-, ( $\alpha$ S)- (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 4 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2010:1447837 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 154:132766

TITLE: Exceptional Superbasicity of Bis(guanidine) Proton Sponges Imposed by the Bis(secododecahedrane) Molecular Scaffold: a Computational Study

AUTHOR(S): Margetic, Davor; Ishikawa, Tsutomu; Kumamoto, Takuya  
CORPORATE SOURCE: Laboratory for Physical-Organic Chemistry, Division of Organic Chemistry and Biochemistry, Ruder Boskovic Institute, Zagreb, 10001, Croatia

SOURCE: European Journal of Organic Chemistry (2010), (34), 6563-6572, S6563/1-S6563/106  
CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

& Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The exceptional superbasicity of a series of bis(guanidines) with a bis(secododecahedrane) mol. scaffold was found in the course of a computational study. The 3-syn,13-syn-disubstituted bis(secododecahedrane) skeleton ensures that nitrogen lone pairs of electrons are in close proximity, and the rigid framework of the polycyclic cage guarantees acid/base properties similar to those of proton sponges. Amine functionalization with alkyl substituents, imines, and guanidines leads to high basicity. Based on DFT computations, bis(guanidine)-bis(secododecahedrane) proton sponges with a (1,3-dimethylimidazolidin-2-ylidene)amino moiety are predicted to have very high basicities, both in the gas phase and acetonitrile. This skeleton provides the highest proton affinity (PA) value among all the aliphatic proton sponges reported (288.7 kcal mol<sup>-1</sup>, whereas the gas-phase basicity is 284.3 kcal mol<sup>-1</sup>, at the B3LYP/6-311+G\*\*//B3LYP/6-31G\* level). In acetonitrile the calculated PA is 319.4 kcal mol<sup>-1</sup> and the estimated pKa is 38.5. Substitution of bis(secododecahedrane) with the intrinsically more basic nitrogen functionalities increases the PA to 316.3 kcal mol<sup>-1</sup> and the pKa to 46.

IT 1261062-12-7

RL: PRP (Properties)

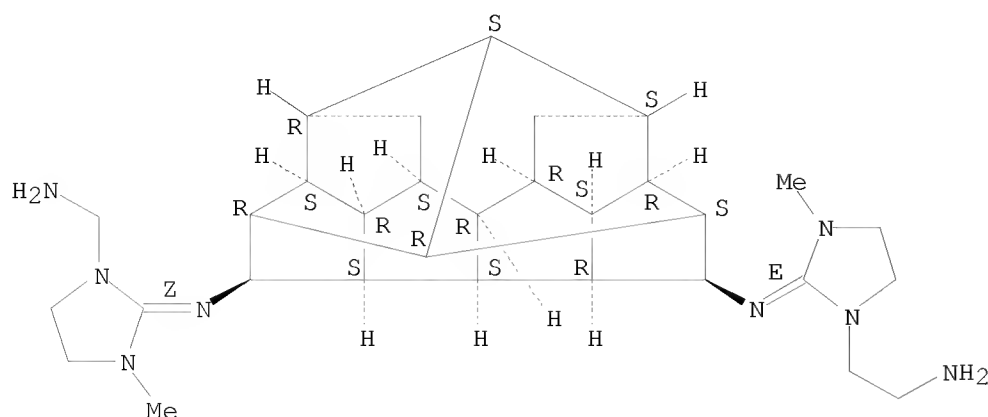
(exceptional superbasicity of bis(guanidine) proton sponges imposed by the bis(secododecahedrane) Mol. scaffold)

RN 1261062-12-7 CAPLUS

CN 2,7,3,6-Ethanediyliidenedipentaleno[1,6-ab:1',6'-ef]pentalene-1,8-diamine, N1-[1-(2-aminoethyl)-3-methyl-2-imidazolinyliidene]-N8-[1-(aminomethyl)-3-methyl-2-imidazolinyliidene]octadecahydro-, stereoisomer (CA INDEX NAME)

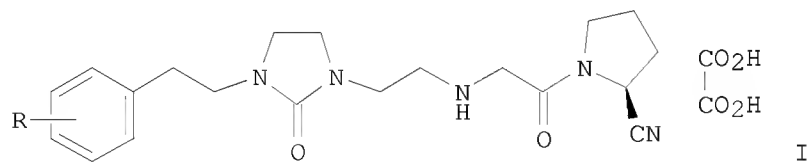
Relative stereochemistry.

Double bond geometry as shown.



OS.CITING REF COUNT: 2 THERE ARE 2 CAPLUS RECORDS THAT CITE THIS RECORD (2 CITINGS)  
 REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2009:1554838 CAPLUS <<LOGINID::20111214>>  
 DOCUMENT NUMBER: 152:262611  
 TITLE: Synthesis and Evaluation of Novel Compounds as Potent Dipeptidyl Peptidase IV Inhibitors  
 AUTHOR(S): Wang, Liutang; Zhang, Bin; Ji, Jianxin; Li, Bogang; Yan, Jufang; Zhang, Weiyu; Wu, Yong; Wang, Xuechao; Hou, Hui  
 CORPORATE SOURCE: West China School of Pharmacy, Sichuan University, Chengdu, 610041, Peop. Rep. China  
 SOURCE: Synthetic Communications (2010), 40(1), 52-57  
 CODEN: SYNCAV; ISSN: 0039-7911  
 PUBLISHER: Taylor & Francis, Inc.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 152:262611  
 GI



AB A series of new 2-cyanopyrrolidine derivs. I [R = H, 4-F, 3-MeO, etc.] with constrained imidazolidin ring were synthesized, Their structures were confirmed by 1H NMR spectroscopy and/or mass spectrometry, and their activities were evaluated in vitro. They were proven to possess submicromolar inhibitory activities against dipeptidyl peptidase IV.  
 IT 1145965-96-3P 1207841-08-4P 1207841-10-8P  
 1207841-12-0P 1207841-14-2P 1207841-16-4P

1207841-18-6P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and evaluation of cyanopyrrolidine derivs. as dipeptidyl peptidase IV inhibitors)

RN 1145965-96-3 CAPLUS

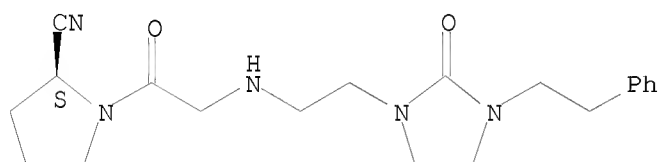
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[2-oxo-3-(2-phenylethyl)-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 1145965-78-1

CMF C20 H27 N5 O2

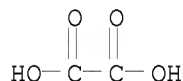
Absolute stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



L5 ANSWER 6 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2009:603998 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 151:148210

TITLE: Synthesis and evaluation of structurally constrained imidazolidin derivatives as potent dipeptidyl peptidase IV inhibitors

AUTHOR(S): Wang, Liutang; Zhang, Bin; Ji, Jianxin; Li, Bogang; Yan, Jufang; Zhang, Weiyu; Wu, Yong; Wang, Xuechao

CORPORATE SOURCE: West China School of Pharmacy, Sichuan University, Chengdu, 610041, Peop. Rep. China

SOURCE: European Journal of Medicinal Chemistry (2009), 44(8), 3318-3322

CODEN: EJMCA5; ISSN: 0223-5234

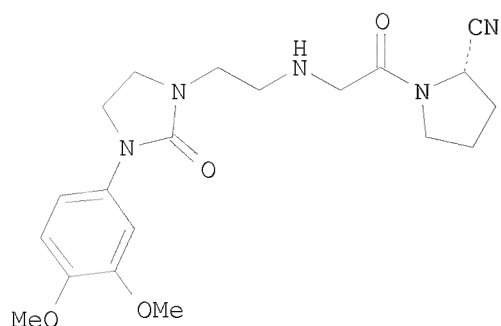
PUBLISHER: Elsevier Masson SAS

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 151:148210

GI



AB To find potent and selective inhibitors of dipeptidyl peptidase IV (DPP-IV), a series of 2-cyanopyrrolidine derivs. with constrained imidazolidine ring was synthesized and their activities against DPP-IV were tested. Most of them exhibited submicromolar inhibitory activities against DPP-IV. The most potent compound among these is (S)-1-(2-(2-(3-(3,4-dimethoxyphenyl)-2-oxoimidazolidin-1-yl)ethyl)amino)acetylpyrrolidine-2-carbonitrile (I), which is a 2 nM DPP-IV inhibitor.

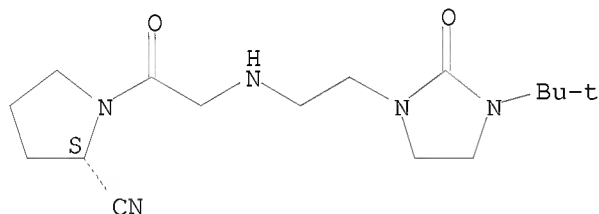
IT 1145965-57-6P 1145965-60-1P 1145965-65-6P  
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and dipeptidyl peptidase IV inhibitory activity of cyanopyrrolidine derivs. with constrained imidazolidine ring)

RN 1145965-57-6 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1,1-dimethylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

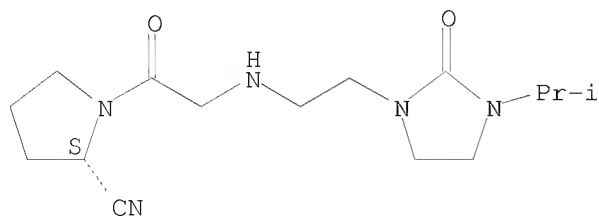
Absolute stereochemistry.



RN 1145965-60-1 CAPLUS

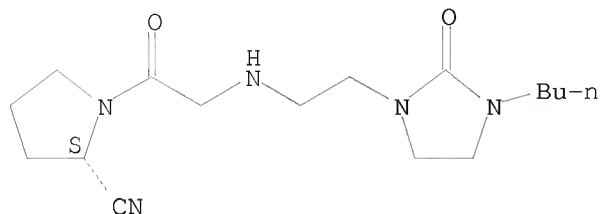
CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1-methylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 1145965-65-6 CAPLUS  
 CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-(3-butyl-2-oxo-1-imidazolidinyl)ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

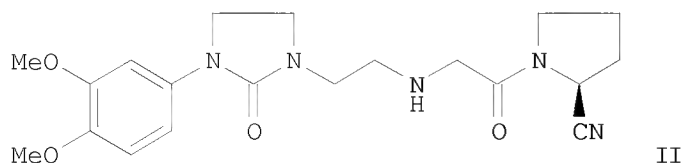
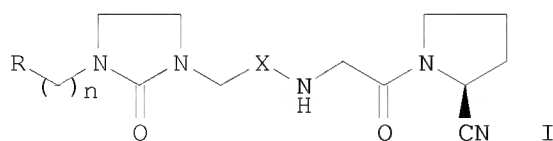


OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD (1 CITINGS)  
 REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 7 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
 ACCESSION NUMBER: 2009:406944 CAPLUS <<LOGINID::20111214>>  
 DOCUMENT NUMBER: 150:448319  
 TITLE: Preparation of N-substituted pyrrolidine derivatives as DPP-IV inhibitors for treating and/or preventing diabetes mellitus  
 INVENTOR(S): Wang, Xuechao; Wang, Liutang; Zhang, Bin; Hou, Hui; He, Zhaoquan; Yan, Jufang; Cen, Guodong; Zhang, Weiyu  
 PATENT ASSIGNEE(S): Chengdu Diao Pharmaceutical Group Co., Ltd., Peop. Rep. China  
 SOURCE: Faming Zhuanli Shenqing, 26pp.  
 CODEN: CNXXEV  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Chinese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 101397294	A	20090401	CN 2008-10161373	20080923
PRIORITY APPLN. INFO.:			CN 2007-10050091	A 20070924
OTHER SOURCE(S):			CASREACT 150:448319; MARPAT 150:448319	

GI



AB The title N-substituted pyrrolidine (Gly-Pro dipeptide) derivs. I [wherein n = 0-3; X = CO, CH<sub>2</sub>, or a bond; R = (un)substituted alkyl, Ph, alkyl, pyridyl, pyridazinyl, pyrazinyl, imidazolyl, pyrazolyl, thiazolyl, etc.] or pharmaceutically acceptable salts thereof were prepared as inhibitors of dipeptidyl peptidase IV (DPP-IV) for treating and/or preventing diabetes mellitus, glucose tolerance disorder, autoimmune diseases, and inflammation. For example, II-oxalate was prepared in a multi-step synthesis. II-oxalate showed inhibitory activity with IC<sub>50</sub> of 0.002  $\mu$ M against DPP-IV. Formulations as tablets and capsules were described.

IT 1145965-56-5P 1145965-57-6P 1145965-60-1P  
 1145965-65-6P 1145965-70-3P 1145965-71-4P  
 1145965-78-1P 1145965-82-7P 1145965-86-1P  
 1145965-92-9P 1145965-96-3P 1145966-03-5P  
 1145966-04-6P 1145966-06-8P

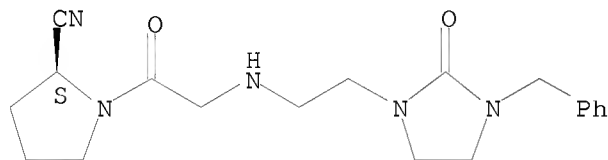
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of N-substituted pyrrolidine derivs. as DPP-IV inhibitors for treating and/or preventing diabetes mellitus)

RN 1145965-56-5 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[2-oxo-3-(phenylmethyl)-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

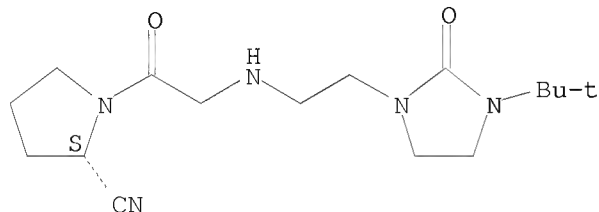
Absolute stereochemistry.



RN 1145965-57-6 CAPLUS

CN 2-Pyrrolidinecarbonitrile, 1-[2-[[2-[3-(1,1-dimethylethyl)-2-oxo-1-imidazolidinyl]ethyl]amino]acetyl]-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



L5 ANSWER 8 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN

ACCESSION NUMBER: 2008:1210838 CAPLUS <<LOGINID::20111214>>

DOCUMENT NUMBER: 149:448395

TITLE: 3-Imidazolylindoles for treatment of proliferative diseases and their preparation



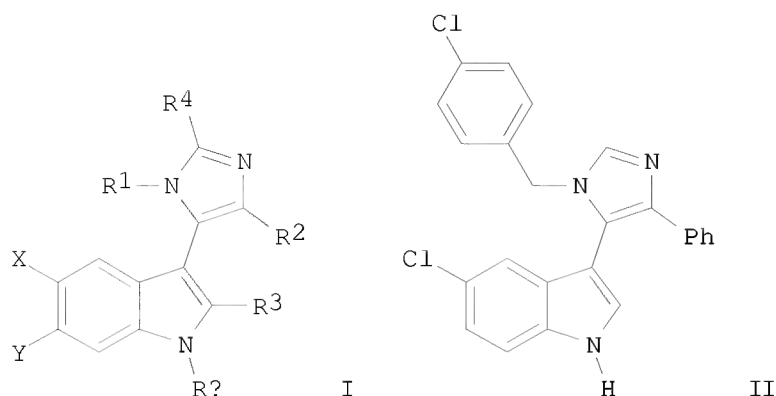
INVENTOR(S): Boettcher, Andreas; Buschmann, Nicole; Furet, Pascal;  
Groell, Jean-Marc; Kallen, Joerg; Hergovich Lisztwan,  
Joanna; Masuya, Keiichi; Mayr, Lorenz; Vaupel, Andrea  
PATENT ASSIGNEE(S): Novartis A.-G., Switz.  
SOURCE: PCT Int. Appl., 260pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008119741	A2	20081009	WO 2008-EP53667	20080327
WO 2008119741	A3	20081204		
W: AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				
AU 2008234954	A1	20081009	AU 2008-234954	20080327
CA 2682483	A1	20081009	CA 2008-2682483	20080327
AR 65860	A1	20090708	AR 2008-101262	20080327
KR 2009122403	A	20091127	KR 2009-7022526	20080327
EP 2142535	A2	20100113	EP 2008-735532	20080327
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LI, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, AL, BA, MK, RS				
JP 2010522723	T	20100708	JP 2010-500280	20080327
ZA 2009006210	A	20100526	ZA 2009-6210	20090908
CR 11019	A	20091020	CR 2009-11019	20090909
IN 2009DN05959	A	20100611	IN 2009-DN5959	20090916
MX 2009010413	A	20091020	MX 2009-10413	20090928
US 20100125064	A1	20100520	US 2009-593721	20090929
US 8053457	B2	20111108		
CN 101679382	A	20100324	CN 2008-80017611	20091126
PRIORITY APPLN. INFO.:			EP 2007-105269	A 20070329
			WO 2008-EP53667	W 20080327

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 149:448395; MARPAT 149:448395

GI



AB The invention relates to 3-heterocyclyl indolyl compds. of formula I, which are capable of inhibiting the interaction between p53, or variants thereof, and MDM2 and/or MDM4, or variants thereof, resp. Due to their activity, the compds. are useful in the treatment of various disorders and diseases mediated by the activity of MDM2 and/or MDM4, or variants thereof. Compds. of formula I wherein R1 and R2 are independently (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted aryl and (un)substituted heterocyclyl; R3 is H, halo, (un)substituted alkyl, (un)substituted alkenyl, (un)substituted alkynyl, (un)substituted aryl, carboxy, cyano, etc.; R4 is H, (un)substituted alkyl and acyl; X is H, C1-7 (halo)alkyl, C1-7 alkoxy, halo and CN; Y is C1-7 (halo)alkyl, C1-7 alkoxy, halo and CN; and their tautomers, N-oxides and salts thereof, are claimed. Example compound II was prepared by formylation of 6-chloro-1H-indole the resulting 6-chloro-1H-indole-3-carboxaldehyde underwent cyclization with 4-chlorobenzylamine and 1-(isocyanophenylmethanesulfonyl)-4-methylbenzene to give compound II. All the invention compds. were evaluated for their MDM2 and MDM4 inhibitory activity (some data given).

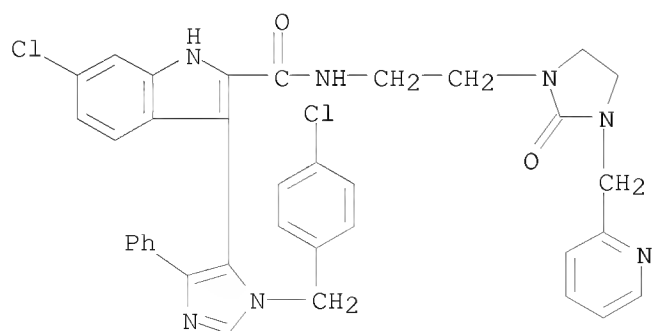
IT 1067657-35-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of imidazolyliindoles as MDM2 and MDM4 inhibitors useful in the treatment of proliferative diseases)

RN 1067657-35-5 CAPLUS

CN 1H-Indole-2-carboxamide, 6-chloro-3-[1-[(4-chlorophenyl)methyl]-4-phenyl-1H-imidazol-5-yl]-N-[2-[2-oxo-3-(2-pyridinylmethyl)-1-imidazolidinyl]ethyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 12 THERE ARE 12 CAPLUS RECORDS THAT CITE THIS  
RECORD (22 CITINGS)

L5 ANSWER 9 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
ACCESSION NUMBER: 2008:1157741 CAPLUS <<LOGINID::20111214>>  
DOCUMENT NUMBER: 149:402368  
TITLE: Preparation of phthalazinone derivatives for use as  
PARP inhibitors  
INVENTOR(S): Menear, Keith Allan; Hummersone, Marc Geoffrey; Gomez,  
Sylvie; Javaid, Muhammad Hashim; Martin, Niall  
Morrison Barr; Kerrigan, Frank  
PATENT ASSIGNEE(S): Kudos Pharmaceuticals Limited, UK; Maybridge Limited  
SOURCE: PCT Int. Appl., 103pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2008114023	A2	20080925	WO 2008-GB990	20080320
WO 2008114023	A3	20081113		
W:	AE, AG, AL, AM, AO, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, NO, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

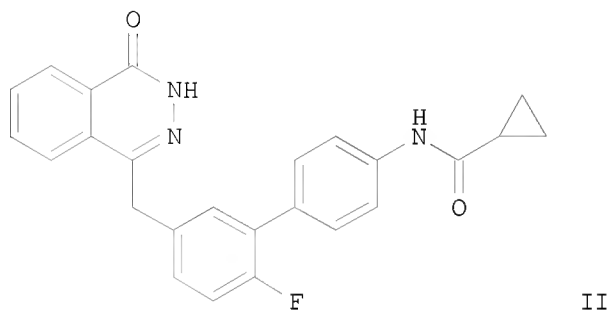
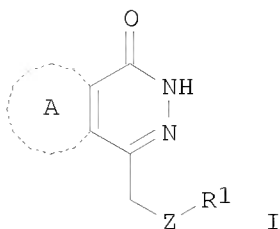
US 20080280910 A1 20081113 US 2008-51219 20080319

PRIORITY APPLN. INFO.: US 2007-896340P P 20070322

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 149:402368; MARPAT 149:402368

GI



AB Title compds. I [Ring A = (un)substituted aromatic or cyclohexene ring; Z = heteroaryl; R1 = (un)substituted aryl bound to Z by a C-C bond; with provisions], and their pharmaceutically acceptable salts, are prepared and disclosed as PARP inhibitors. Thus, e.g., II was prepared by coupling of 4-(3-bromo-4-fluorobenzyl)-2H-phthalazin-1-one (preparation given) with (4-aminophenyl)boronic acid followed by amidation with cyclopropanecarboxylic acid. Select I were evaluated in PARP inhibition assays, e.g., II demonstrated an IC50 value of 0.057  $\mu$ M.

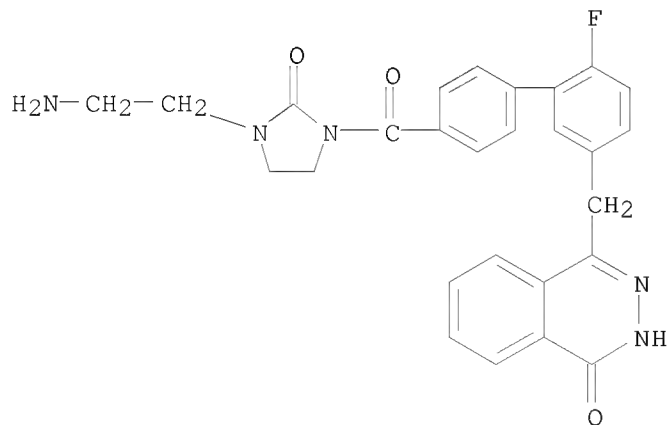
IT 1062291-39-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of phthalazinone derivs. for use as PARP inhibitors)

RN 1062291-39-7 CAPLUS

CN 1(2H)-Phthalazinone, 4-[[4'-[[3-(2-aminoethyl)-2-oxo-1-imidazolidinyl]carbonyl]-6-fluoro[1,1'-biphenyl]-3-yl]methyl]- (CA INDEX NAME)



OS.CITING REF COUNT: 1 THERE ARE 1 CAPLUS RECORDS THAT CITE THIS RECORD  
(1 CITINGS)

L5 ANSWER 10 OF 61 CAPLUS COPYRIGHT 2011 ACS on STN  
ACCESSION NUMBER: 2007:564518 CAPLUS <<LOGINID::20111214>>  
DOCUMENT NUMBER: 147:9799  
TITLE: Preparation of piperidine derivatives as antitumor agents  
INVENTOR(S): Collibee, Scott; Yang, Zhe; Ashcraft, Luke; Bergnes, Gustave; Morgan, Bradley P.; Morgans, David J., Jr.  
PATENT ASSIGNEE(S): Cytokinetics, Inc., USA  
SOURCE: PCT Int. Appl., 191pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
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PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007059323	A2	20070524	WO 2006-US44753	20061115
WO 2007059323	A3	20071227		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			
US 20070161674	A1	20070712	US 2006-600684	20061115
US 7572814	B2	20090811		
AR 58839	A1	20080227	AR 2006-105001	20061115
EP 1962846	A2	20080903	EP 2006-837964	20061115
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, MK, RS			
PRIORITY APPLN. INFO.:			US 2005-737226P	P 20051115
			WO 2006-US44753	W 20061115

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT

OTHER SOURCE(S): CASREACT 147:9799; MARPAT 147:9799  
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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Piperidine derivs. I, wherein X is chosen from =O and =N-OR, where R is selected from hydrogen and alkyl, provided that at least one =X is =O, R1 is chosen from hydrogen, alkyl, cycloalkyl, heterocycloalkyl, aryl and heteroaryl; R2 is chosen from aryl, heterocycloalkyl, alkyl, cycloalkyl, heteroaryl, alkoxy, hydroxy, and amino; R3 is chosen from hydrogen and alkyl; R4 is chosen from hydrogen, alkyl, heterocycloalkyl, acyl, aryl, heteroaryl, amino-carbonyl, sulfonyl, alkoxycarbonyl, and cycloalkyl; R5 is chosen from hydrogen and alkyl; and R6 is chosen from aryl,

heterocycloalkyl, alkyl, cycloalkyl, heteroaryl, alkoxy, hydroxy, and amino, were prepared via cyclocondensation of methylene derivs. with primary amines, and used for treating cellular proliferative diseases. Thus, cyclocondensation of methylene II with benzylamine gave piperidine III, which was used as intermediate in synthesis of title compds. Thus, (cis,trans)-1-(2-hydroxyethyl)-4-phenyl-5-(phenyl-carbonyl) (3-piperidyl)phenyl-ketone was prepared and tested in vitro and in nude mice as antitumor agent. In vitro potency of chemical entities provided herein can be determined, for example, by assaying human ovarian cancer cells (SKOV3) for viability following a 72-h exposure to a 9-point dilution series of compound. The composition of title compds. is formulated in a form chosen from injectable fluids, aerosols, creams, gels, tablets, pills, capsules, syrup; ophthalmic solns., and patches. Certain of the chemical entities described herein were evaluated for in vivo activity against SKOV-3 human ovarian carcinoma in a tumor growth delay (TGD) study. The study utilized eight groups (n = 8) of athymic nude mice bearing established (63-144 mm<sup>3</sup>) SKOV-3 tumors on day 1, and included a vehicle-treated tumor growth control group and a reference group treated with paclitaxel (30 mg/kg i.v. qod x 5). Title compds. were evaluated at doses of 300 or 150 mg/kg administered i.p. once daily and at 150 mg/kg administered i.p. twice daily. The 250 and 500 mg/kg once daily treatments produced 15 and 58 % TGD, resp., which was statistically significant activity at 500 mg/kg. The 250 mg/kg twice daily treatment produced 57 % TGD, which was statistically significant activity.

IT 937713-50-3P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of piperidine derivs. as antitumor agents via cyclocondensation of methylene derivs. with primary amines)

RN 937713-50-3 CAPLUS

CN 2-Imidazolidinone, 1-[2-(dimethylamino)ethyl]-3-[2-[(3R,5S)-4-(3-fluoro-2-methylphenyl)-3,5-bis(3-hydroxybenzoyl)-1-piperidinyl]ethyl]-, rel- (CA INDEX NAME)

Relative stereochemistry.

